

Critical Scaling Properties at the Superfluid Transition of ^4He in Aerogel

Marios Nikolaou,¹ Mats Wallin,¹ and Hans Weber²

¹*Department of Theoretical Physics, Royal Institute of Technology, AlbaNova, SE-106 91 Stockholm, Sweden*

²*Department of Physics, Luleå University of Technology, SE-971 87 Luleå, Sweden*

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We study the superfluid transition of ^4He in aerogel by Monte Carlo simulations and finite size scaling analysis. Aerogel is a highly porous silica glass, which we model by a diffusion limited cluster aggregation model. The superfluid is modeled by a three dimensional XY model, with excluded bonds to sites on the aerogel cluster. We obtain the correlation length exponent $\nu = 0.73 \pm 0.02$, in reasonable agreement with experiments and with previous simulations. For the heat capacity exponent α , both experiments and previous simulations suggest deviations from the Josephson hyperscaling relation $\alpha = 2 - d\nu$. In contrast, our Monte Carlo results support hyperscaling with $\alpha = -0.2 \pm 0.05$. We suggest a reinterpretation of the experiments, which avoids scaling violations and is consistent with our simulation results.

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Experiments on ^4He immersed in ultralight aerogel, forming highly porous fractal structures, have demonstrated new universality classes of the superfluid phase transition [1, 2]. Striking deviations of the critical exponents from the bulk lambda transition appear to arise due to fractal correlations in the aerogel, but the details are not well understood. Furthermore, the new critical exponents tend to violate common scaling laws, such as the Josephson hyperscaling relation. A theoretical study of the unusual scaling properties of the superfluid transition in fractal random media is motivated in order to better understand these surprising results.

Experiments on helium in aerogel use ultralight aerogel samples with a highly porous structure that consists of silica strands of about 5 nm in diameter and a distance between neighboring strands of up to 200 nm [2]. The porosity can be varied in the fabrication process. Small-angle x-ray scattering indicates a fractal structure extending from a couple of nanometers up to more than 100 nm [3]. The superfluid density of the ^4He has been measured by a torsional oscillator technique, and the heat capacity by an ac heating method [2]. The superfluid density was found to vanish at the transition as a power law $\rho_s = \rho_0|t|^\zeta$, where $t = 1 - T/T_c$ and $\zeta \approx 0.79$ for $m = 5\%$ volume fraction of aerogel, $\zeta \approx 0.76$ for $m = 2\%$, and $\zeta \approx 0.72$ for $m = 0.5\%$. These values are significantly greater than $\zeta \approx 0.67$ found in bulk ^4He . The heat capacity has a peak at $T = T_c$ that was fitted to the form $C = A_\pm|t|^{-\alpha_\pm} + B$, giving $\alpha_+ \neq \alpha_-$. Alternatively, assuming that $\alpha_+ = \alpha_- = \alpha$ gives $\alpha \approx -0.57$ for $m = 5\%$ aerogel, $\alpha \approx -0.39$ for $m = 2\%$, and $\alpha \approx -0.13$ for $m = 0.5\%$ [2]. Surprisingly, these exponents depend on the aerogel porosity, and deviate considerably from the value obtained from the Josephson hyperscaling relation, $\alpha = 2 - d\nu$, with $d = 3$ and $\nu = \zeta$.

The ^4He transition in aerogel has been studied by computer simulation in Refs. [4, 5], and we follow many aspects of these works. Moon and Girvin [4] studied a

three dimensional (3D) XY model with aerogel modeled as a connected percolation fractal cluster with fractal dimension $D_f \approx 2.5$. They obtained the expected scaling behavior of the superfluid density, i.e., $\rho_s \sim \xi^{2-d}$ with $d = 3$, and a correlation length that diverges as $\xi \sim |T - T_c|^{-\nu}$ with exponent $\nu \approx 0.722$, in agreement with experiments [2]. However, they did not study the unusual heat capacity exponents. Vásquez et al. [5] also studied a 3D XY model, but with aerogel modeled with a diffusion limited cluster aggregation (DLCA) algorithm, generating a fractal cluster with dimension $D_f \approx 1.8$ [6]. They find porosity dependent exponents similar to those from the experiments. Specifically, the heat capacity exponent displays a similar violation of hyperscaling as obtained from experiments.

In this Letter we study the superfluid transition in aerogel by Monte Carlo (MC) simulations and finite size scaling analysis, using a more extensive disorder averaging and larger system sizes than in previous simulations. In contrast to results from experiments and earlier simulations, we obtain critical exponents that are both porosity independent and obey usual scaling laws. In particular, our MC data is consistent with the Josephson hyperscaling relation. We reanalyze the experimental data for the heat capacity from Ref. [2] in light of our new scaling results, and argue that the formula $C = A_\pm|t|^{-\alpha_\pm} + B$ used in the previous data analysis may not directly apply for this problem. We present an alternative analysis that leads to consistency between experiments and our simulation results.

DLCA model. – Following Ref. [5], we model the aerogel using a DLCA algorithm [7, 8]. We consider a simple cubic lattice with $L \times L \times L$ sites and periodic boundary conditions in all directions. As a first step mL^3 “particles” are distributed on random lattice sites, where m is the volume fraction of the aerogel. Particles on nearest neighbor lattice sites form clusters, whose structure is kept fixed. Clusters are allowed to diffuse by rigid

translations, using an iterative DLCA algorithm [9]. If two clusters meet they connect irreversibly and form a larger cluster. The iteration continues until a single cluster remains, which is used to model the aerogel, and plays the role of correlated disorder for the helium. The aerogel volume fractions considered here are $m = 5\%$ and $m = 10\%$.

3D XY model. – The universal properties of the superfluid transition of ^4He are captured by the 3D XY model given by

$$H = - \sum_{\langle i,j \rangle} J_{ij} \cos(\theta_i - \theta_j), \quad (1)$$

where $\langle i, j \rangle$ denotes nearest neighbor sites. The coupling constant J_{ij} is set to $J = 1$ between pairs of ^4He sites, and $J = 0$ if one or both lattice sites belong to the DLCA cluster. The excluded bonds act like quenched disorder for the 3D XY model, and θ_i is the phase of the superfluid order parameter at site i occupied by helium.

Monte Carlo simulations. – Our MC simulations use the collective Wolff update method [10], combined with the temperature exchange method [11], which reduces critical slowing down of the simulation. An exchange update attempt was performed after every ten Wolff cluster updates. For each random bond realization we discard between 2×10^4 and 2×10^5 Wolff clusters to approach equilibrium, depending on system size, followed by the same number of updates collecting data. In the temperature exchange method we simulate a set of different temperatures in parallel, and allow MC moves exchanging the temperatures between the different configurations. The results were averaged over 5×10^3 DLCA clusters for $L \leq 50$, and for 2.5×10^3 clusters for $L \geq 60$. We carefully checked for convergence of the simulation by increasing the number of initial discarded update steps until stable results were obtained.

Calculated quantities and finite size scaling relations.

– The superfluid density ρ_s is proportional to the helicity modulus Y , which gives the increase in free energy density as $\Delta f = \frac{1}{2} Y \Delta^2$ in the presence of a uniform phase twist Δ imposed across the system, here taken in the x direction [12]. The helicity modulus is then given by [13]

$$Y(T, L) = \frac{1}{L^3} \left[\left\langle - \sum_j J_j^x \cos(\theta_{j+\hat{e}_x} - \theta_j) \right\rangle \right. \\ \left. - \frac{1}{L^3 T} \left[\left\langle \left(\sum_j J_j^x \sin(\theta_{j+\hat{e}_x} - \theta_j) \right)^2 \right\rangle \right] \right], \quad (2)$$

where $J_j^x = J_{j+\hat{e}_x, j}$. Here $\langle \dots \rangle$ denotes thermal average, and $[\dots]$ denotes average taken over different realizations of DLCA clusters.

In order to analyze MC data for finite systems of size L^3 , we start from the finite size scaling relation for the singular part of the free energy density, $f_s/T = L^{-d} \tilde{f}_\pm(L/\xi)$, where $d = 3$, \tilde{f}_\pm are scaling functions, and

$\xi \sim |T - T_c|^{-\nu}$ is the correlation length [14]. The corresponding scaling result for a phase gradient is $\Delta = L^{-1} \tilde{\Delta}_\pm(L/\xi)$. The helicity modulus becomes $Y \sim L^{2-d}$, or, alternatively, $Y \sim |T - T_c|^\zeta$ [12] with $\zeta = (d - 2)\nu$. For $d = 3$ the finite size scaling relation becomes [4]

$$LY/T = (1 + aL^{-\omega}) \tilde{Y}(L^{1/\nu} t), \quad (3)$$

where \tilde{Y} is a scaling function to be determined below from MC data, and $t = T - T_c$. The term $aL^{-\omega}$ is an amplitude correction to scaling that will be discussed below [15].

The Josephson hyperscaling relation for the heat capacity exponent, $\alpha = 2 - d\nu$, follows from $c \sim \partial^2 f_s / \partial T^2 \sim \partial^2 t^{d\nu} / \partial t^2 \sim t^{d\nu-2} = t^{-\alpha}$ [14]. The heat capacity is given by $c = [\langle H^2 \rangle - \langle H \rangle^2] / (L^3 T^2)$, and the finite size scaling relation is [16]

$$c = L^{\alpha/\nu} \tilde{c}(L^{1/\nu} t) + b, \quad (4)$$

where b represents the nonsingular, analytic contribution to the heat capacity, which depends on temperature but not system size. Since we focus on a narrow temperature interval around the transition, we take b to be constant. Alternatively, the scaling function can be determined directly by eliminating b :

$$\tilde{c}(x) = \frac{c(x, L_1) - c(x, L_2)}{L_1^{\alpha/\nu} - L_2^{\alpha/\nu}}, \quad (5)$$

where x is the scaling variable $L^{1/\nu} t$ and L_1, L_2 denote two different system sizes. These two formulas gave the same results for the critical exponents.

Results. – Figure 1 shows MC data for the heat capacity c (main figure) and the dimensionless helicity modulus LY/T (inset) vs temperature T for a set of different system sizes L for an aerogel volume fraction of $m = 5\%$. According to the scaling relation Eq. (3), the dominant L dependence for the helicity modulus at $T = T_c$ is $Y \sim L^{-1}$, showing that the superfluid transition temperature T_c is where all data curves for LY/T for different system sizes L intersect. However, a close examination of the data curves for Y in Fig. 1 reveals a small systematic drift in the intersection temperatures between successive pairs of system sizes, which complicates an accurate determination of T_c . The drift can be included in the scaling analysis by assuming an amplitude correction to scaling of the form included above in Eq. (3). We found that varying ω in the interval from 0.6 to 1 leads to practically indistinguishable fits to the MC data, with nearly the same values for the other exponents. The precision of our MC data is not enough for a more accurate estimate of ω , and the results shown below are for the choice $\omega = 1$. For the heat capacity no correction to scaling was found to be necessary.

The following method produces a finite size data collapse of MC data for the helicity modulus by fitting

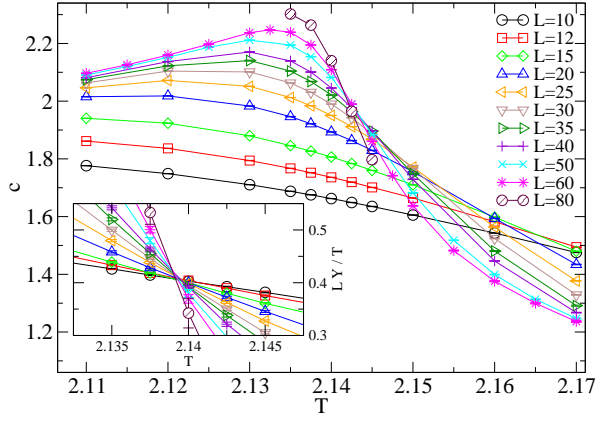


FIG. 1: (color online) MC data for the heat capacity c (main figure) and the dimensionless helicity modulus LY/T (inset) as a function of temperature T for different system sizes L , with $m = 5\%$ aerogel volume fraction.

to Eq. (3). The χ^2 value of the fit is obtained as $\chi^2 = (1/n) \sum_{i,j} \int dx [\tilde{Y}_i(x) - \tilde{Y}_j(x)]^2$, where i, j refer to n pairs of system sizes L_i, L_j . The integrals are evaluated using cubic spline interpolation at 20 evenly spaced points within the x interval in which the pair of functions in the integrand overlap. The fit parameters are determined by minimizing χ^2 over a fine multidimensional grid of values, whose resolution is finer than the error estimates on the parameters. Data points at small values of Y with poor statistics are excluded from the fits. A similar procedure is used to fit Eq. (4) to the heat capacity data. We tried both independent scaling fits for Y and c , and joint fits to scale both quantities simultaneously, which we found to be more stable.

To determine the critical exponents ν and α we attempt some different approaches. We first assume that the hyperscaling relation $\alpha = 2 - d\nu$ is valid, which leaves the fit parameters T_c, ν, a, b . The result of joint fits of Eqs. (3) and (4) to MC data is shown in Fig. 2 for $m = 5\%$. As seen in the figure the fit produces good data collapses both for Y and for c . The fit parameters for $m = 5\%$ are: $T_c = 2.1385 \pm 0.0005$, $\nu = 0.73 \pm 0.02$, $a = -1.9$, $b = 2.85$, and for $m = 10\%$ (data not shown): $T_c = 2.0450 \pm 0.0005$, $\nu = 0.73 \pm 0.02$, $a = -2.0$, $b = 2.6$. Error bars are estimated from the variation in the parameter values upon varying the range of system sizes included in the fits. We observe a slight tendency for the exponents to drift towards the 3D XY results upon increasing the system sizes included in the scaling fits, but larger system sizes would be required to study this effect further. The values of T_c are close to the value $T_c \approx 2.203$ for the pure 3D XY model, which is expected since the DLCA cluster fills only a tiny fraction of the entire system volume. The values of ν for 5% and 10% aerogel closely agree with each other, and we get the corresponding heat capacity exponent $\alpha = 2 - 3\nu = -0.20 \pm 0.05$, indepen-

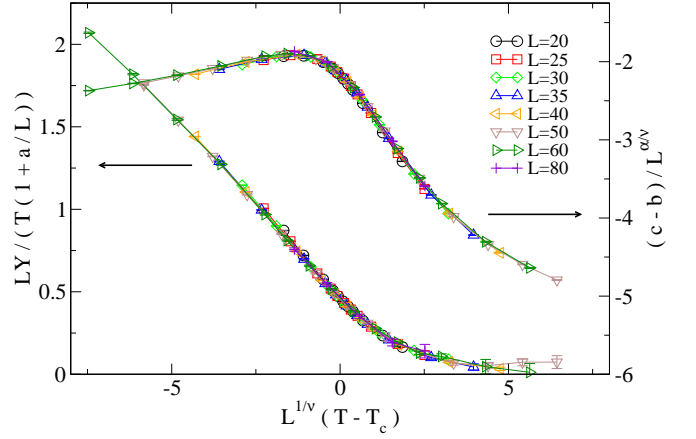


FIG. 2: (color online) Finite size scaling data collapses of MC data showing the scaling functions for the helicity modulus Y and the heat capacity c for $m = 5\%$. The data collapses giving the scaling functions are obtained from a joint fit to Eqs. (3) and (4) for system sizes $L \geq 20$, assuming that α is given by the hyperscaling relation $\alpha = 2 - d\nu$.

dent of the aerogel porosity. We also tried joint scaling fits without assuming the hyperscaling relation for α , but instead treating ν and α as independent fit parameters, with similar results. On the other hand, using the parameter values suggested by the experiments [2] gives a good fit to the helicity modulus, but a very poor fit to the heat capacity data. Thus, from fits to our MC data we conclude that the exponents are porosity independent and obey hyperscaling, in contrast to suggestions in Refs. [2, 5].

Comparison with experiments. – Here we compare our critical exponents to the experimental results in Ref. [2]. Our scaling of the helicity modulus gives the correlation length exponent $\nu \approx 0.73$, which compares quite well with the experimental values $\nu = 0.72 - 0.79$ from torsional oscillator measurements of the superfluid density. However our heat capacity exponent $\alpha \approx -0.20$ is far from the experimental values $\alpha = -0.39$ for $m = 2\%$ aerogel, and $\alpha = -0.57$ for $m = 5\%$. These results are clearly incompatible.

We now argue that our scaling results can actually describe the universal scaling function probed by the experiment. However, we also suggest that the experimental data contains nonuniversal features that must be included in the data analyses as well. We first assume the presence of a finite cutoff length scale in the experimental system. Figure 3 of Ref. [2] shows that the data for the ^4He transition without any aerogel produces a sharp lambda curve. However, the presence of the aerogel seems to slightly round off the maximum of the heat capacity curves, compared to the sharp peak predicted by the formula $c \sim |T - T_c|^{-\alpha}$. Rounding of the experimental curves therefore seems to be caused by the presence of the aerogel, and suggests a finite length scale that may

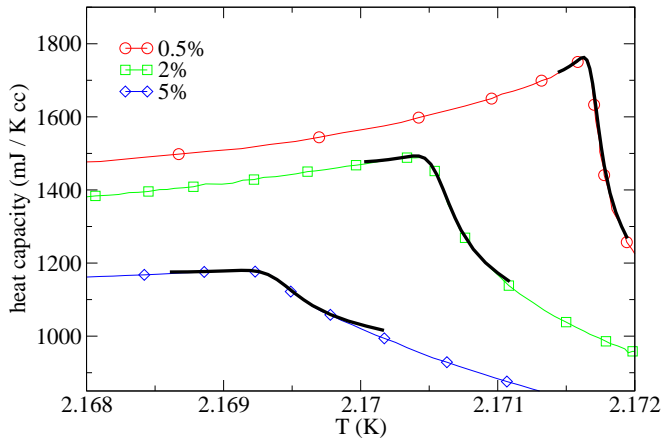


FIG. 3: (color online) Experimental data of the heat capacity for three aerogel volume fractions, 0.5%, 2%, and 5%, reproduced from Ref. [2] (curves with symbols), together with fits to the scaling function (thick curves) given by Eq. (6).

be associated with the typical aerogel pore size.

Further, we argue that the temperature dependence of the superfluid condensate amplitude may contribute to the observed asymmetry of the experimental heat capacity curves around T_c . The fit presented in Ref. [2] to extract α from experiments assumes that only the singular $c \sim |T - T_c|^{-\alpha}$ dependence on T is observed. We propose that this might be too restrictive in cases when α is negative, since the singular temperature dependence does not clearly dominate the temperature variation as when $\alpha \gtrsim 0$. We include the regular temperature dependence of the amplitude by a linear approximation of the form $A = A_0 + A_1 T$, where A_0, A_1 are constants [17]. This gives

$$c(T) = (A_0 + A_1 T) \left\{ L^{\alpha/\nu} \tilde{c}[L^{1/\nu}(T - T_c)] + b \right\}, \quad (6)$$

where the scaling function \tilde{c} is determined in Fig. 2. To fit Eq. (6) to experiments we assume $\alpha = -0.20$, $\nu = 0.73$ and use L, b, A_0, A_1 as fit parameters. The results of the fits are shown in Fig. 3. The fit parameters are: $m = 5\%$: $L = 835, b = 5.03, A_0 = 13592, A_1 = -6150$; $m = 2\%$: $L = 1107, b = 2.84, A_0 = 65914, A_1 = -30098$; $m = 0.5\%$: $L = 1900, b = 1.98, A_0 = 193062, A_1 = -88428$. We thus obtain quite good agreement in a narrow interval around the transition between the experiment of Ref. [2] and a fit to the simulated scaling function, which fulfills hyperscaling. The 5% data curve shows a slight deviation between theory and experiment on the high temperature side of the transition in Fig. 3. This deviation occurs away from the transition temperature, where additional temperature dependencies are expected. Note that the cutoff length depends roughly as $L \sim 1/m^{1/3}$, which is compatible with the interpretation as a crossover related to the typical pore diameter in the aerogel.

Discussion. – From our finite size scaling analysis of

MC data for the 3D XY model in aerogel modeled as DLCA clusters, we obtain a correlation length exponent $\nu \approx 0.73$. This supports the previous conclusion [4, 5] that the universality class of the phase transition in the presence of DLCA clusters deviates from the pure 3D XY universality class, where $\nu \approx 0.671$ [15], even though the possibility of a slow crossover towards the pure 3D XY universality class cannot entirely be ruled out. In contrast to previous results in the literature [2, 5], our results suggest that the critical exponents are independent of porosity and obey the Josephson hyperscaling relation $\alpha = 2 - d\nu$, within the statistical uncertainty of the MC data. We argue that the formula $c = A_{\pm}|T - T_c|^{-\alpha_{\pm}} + B$, used to analyze experiments in Ref. [2] is not directly applicable in this case. We propose an alternative analysis procedure based on our simulation result to fit the experimental heat capacity data at the transition. This fit assumes that the experiment contains signatures of a finite crossover length scale, presumably related to the typical aerogel pore size, and of a temperature dependent superfluid condensate amplitude.

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